## Local Spontaneous Symmetry Breaking for Film System Within Scalar $\phi^4$ Model for Phase Transition

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The difficulty is analysed in evaluating fluctuations in phase transition of finite-size system at temperature far below the critical point. Film system is discussed with one-component order parameter  $\phi^4$  model for phase transition. Non-trivial vacuum state corresponding to minimum Hamiltonian is given approximately for various boundary conditions. It is shown that the spontaneous symmetry breaking plays an important role for such systems, and that perturbative calculations can be done safely when the effect of the vacuum state or the local spontaneous symmetry breaking is taken into consideration.

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Finite-size effects near critical points have been remained over the past two decades to be an important topic of the active research both theoretically and experimentally [1]. Nowadays, the experimental sample are usually so pure and so well shielded from perturbing fields that the correlation length can grow up to several thousand angstroms as the critical point is approached. When one or more dimensions of a bulk system is reduced to near or below a certain characteristic length scale, the associated properties are modified reflecting the lower dimensionality. It is believed that finite-size effects are precursors of the critical behavior of the infinite system and can be exploited to extract the limiting behavior. A central role plays the finite-size scaling behavior predicted by both the phenomenological [2] and renormalization group [3] theories. Those theories allowed a systematic discussion of the finite-size effects and, consequently, form the cornerstone of our current understanding of the way in which the singularities of an infinite system are modified by the finiteness of the system in some or all of the dimensions. Of course, the exact form of scaling functions can't be given in those scaling theories.

In 1985, Brézin and Zinn-Justin (BZ) [4] and Rudnick, Guo and Jasnow (RGJ) [5] developed two field-theoretical perturbation theories for the calculation of the finite-size scaling functions within the  $\phi^4$  model which corresponds to the Ising model. Most applications of these theories to three-dimensional systems have been restricted to T higher than the bulk critical temperature  $T_C$  [6] with a few calculations in region below  $T_C$  [7]. In recent years the  $\phi^4$ and the extended  $\phi^6$  models have been used to investigate the multiplicity fluctuations in the final states for firstand second-order phase transitions of quark gluon plasma [8, 9], under the approximation similar to the so-called zero-mode approximation. However, some limitations exist in the theories of Ref. [4,5]. As pointed out in the first paper in Ref. [10], the theory of BZ is not applicable for  $T < T_C$  and the results from RGJ theory are not quantitatively reliable in the same temperature region since the coefficients of the Gaussian terms in the integrals are negative for those temperatures. In Ref. [11] the order parameter is expanded into sum of eigenfunctions of  $\nabla^2$  for various boundary conditions. Again, the functional integral is turned out into normal integrals. But the fluctuations can be evaluated only for temperature not too far below the critical point. Authors of Ref. [10] tried to avoid the difficulty mathematically, but they failed to account for the origin of the difficulty physically. Although the modified perturbation method in Ref. [10] can be used for both  $T > T_C$  and  $T < T_C$ , the calculation is lengthy and can be done only to the first order in practice. Since one does not know the exact order of values of higher order terms, theoretical results have large uncertainty.

It should be pointed out that all perturbation theories mentioned above are based on Fourier decomposition of the order parameter. This method is natural because the decomposition enables one to transform the functional integral into an infinite product of tractable normal integrals. Although such decomposition has simple physical explanation which is very fruitful for the understanding of properties of infinite systems and can deduce reliable physical results, as in the case of usual field theories in particle physics, it brings about a great deal of calculations for systems with finite-size. This is not surprising. As is well-known, quantities complicated in coordinate space may have simple momentum spectra thus look simpler in momentum space, but those obviously nonzero only in a finite range must have puzzling momentum spectra. Therefore, for the study of properties of finite-size systems, calculations in coordinate space

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might be simpler and more effective. The point here is that one must calculate the complicated functional integral which is very difficult to be evaluated directly.

It should be asked that which physical effect causes the failure of direct perturbative calculation of fluctuations for finite-size system with temperature below  $T_C$ . In our opinion, the real origin of the difficulty lies in the lack of knowledge about the spontaneously symmetry breaking for finite-size systems. It is well-known that an infinite system will have non-zero mean order parameter  $\phi_0$ , which is called vacuum state of the system in this Letter since it corresponds to minimum of the Hamiltonian H, if the temperature is below the critical one, and everyone knows that the difficulty of negative coefficient for the Gaussian term can be overcome by shifting the order parameter,  $\phi \to \phi + \phi_0$ . This phenomenon is known as the spontaneous symmetry breaking because of the fact that  $\phi_0$  does not have the same symmetry as H does. This kind of spontaneous symmetry breaking for infinite system can be called global since the shift  $\phi_0$  is the same for every point in the space. For finite-size system, such a simple shift of the order parameter does not work because of the existence of specific boundary conditions for the systems. Anyway, fluctuations of the system, in their own sense, should be around certain vacuum state which corresponds to minimum Hamiltonian H, and they can be approximated by Gaussian terms in most cases if they are not very large. Thus one sees that the vacuum state plays an determinative role in the study of fluctuations in the phase transitions. For infinite system, the vacuum state  $\phi_0$  is constant and can easily be calculated. But for finite-size systems, the vacuum is surely not constant nor it is easy to be obtained. So, the spontaneous symmetry breaking for finite size system can be called local one. Therefore, the solution for the vacuum state is non-trivial and necessary, and one has reason to hope that the difficulty mentioned above can be overcome once the vacuum state is known.

In this Letter, we first calculate the vacuum states for  $\phi^4$  model of phase transition with one-component order parameter under various boundary conditions. Then, with the vacuum states, the Hamiltonian of the system is reexpressed as Gaussian term and higher order fluctuations of a locally shifted order parameter. And it is shown that the perturbative calculation can be done with the new Hamiltonian for temperatures far below the bulk critical point.

In a  $\phi^4$  model for phase transition with a one-component order parameter, the partition function can be expressed as a functional integral of exponential of the Hamiltonian H of the system

$$Z = \int \mathcal{D}\phi \exp(-H) = \int \mathcal{D}\phi \exp\left\{-\int d^3 x \left[\frac{\gamma}{2}\phi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{u}{4!}\phi^4\right]\right\} , \qquad (1)$$

in which  $\gamma = a(T - T_C)$ , a and u are temperature dependent positive constants,  $\phi$  is the order parameter of the system. In the following, we are limited only to systems of a film with thickness L. Since we are interested only in the temperature region  $T < T_C$  or  $\gamma < 0$ , the Hamiltonian H can be standardized by introducing correlation length  $\xi = \sqrt{-1/\gamma}$ , new order parameter  $\Psi = \phi/\phi_0$  with  $\phi_0 = \sqrt{-6\gamma/u}$  the vacuum state for bulk system, scaled coordinates  $\mathbf{r}' = \mathbf{r}/L$ , and reduced thickness  $l = L/\xi$ , into

$$H = \int d^3x' \frac{L^3 \phi_0^2}{\xi^2} \left[ \frac{1}{2l^2} (\nabla' \Psi)^2 - \frac{1}{2} \Psi^2 + \frac{1}{4} \Psi^4 \right] . \tag{2}$$

From this expression one can get the equation for the vacuum state by  $\frac{\delta H}{\delta \Psi} = 0$ . The vacuum state satisfies

$$\frac{1}{l^2} \frac{d^2 \Psi_0}{dx^2} = -\Psi_0 + \Psi_0^3 \ . \tag{3}$$

In the equation we have used x instead of x' in the range (0, 1) to denote the coordinate along the thickness direction. Derivatives in other directions do not appear in the equation since any state with non-zero derivatives in other directions does not correspond to minimum H. But if the system in fully limited in all directions, last equation should have  $\nabla^2$  in place of  $d^2/dx^2$ . In Ref. [12] last equation is solved analytically for Dirichlet boundary conditions  $\Psi(0) = \Psi(1) = 0$ . The exact solution is

$$\Psi_0(x) = \frac{\sqrt{2k}}{\sqrt{1+k^2}} \operatorname{sn}(2xF(k), k) , \qquad (4)$$

in which k is determined by l through  $l=2\sqrt{1+k^2}F(k)$ . Here, F(k) is the first kind of complete elliptic integral,  $\operatorname{sn}(x,k)$  is elliptic sine function. Unfortunately, no simple compact solution is found yet for other boundary conditions. One can easily see that the main obstacle comes from the nonlinear term  $\Psi^3$  in the differential equation of  $\Psi$ . To find approximate solutions of  $\Psi$  for other boundary conditions, the following method can be used. First of all, we replace  $\Psi^3$  by  $\lambda\Psi$  and get a solution satisfying the same boundary condition. For Dirichlet boundary conditions, the solution is

$$\Psi_0 = A \sin \pi x$$
, and  $\lambda = 1.0 - \pi^2 / l^2$ . (5)

The constant A can be determined by requiring the mean square of the deviation caused by the replacement, i.e., the integral  $\int_0^1 dx (\Psi_0^3 - \lambda \Psi_0)^2$ , to be minimum. Thus one gets

$$\Psi_0(x) = \sqrt{\frac{4}{3} \left(1 - \frac{\pi^2}{l^2}\right)} \sin \pi x \ . \tag{6}$$

Now one can see that the requirement of minimum deviation caused by the replacement is equivalent to retaining  $\sin \pi x$  term but neglecting terms with higher frequency in  $\Psi_0^3$ . Thus, this approximation is equivalent to the standard functional variation method. The virtue of this method is that it can be used more simply and in a step-by-step way. As discussed in Ref. [12], the vacuum state  $\Psi_0 = 0$  if the reduced thickness l of the film is less than  $\pi$ . The existence of minimum reduced thickness of the film implies a shift of the critical temperature for the finite system from the bulk one. The exact solutions and the approximate ones are compared in Fig. 1 for  $l/\pi=1.05$ , 1.10, 1.15, and 1.20. A very good approximation can be seen. For larger l, the same approximative method can be used further after shift  $\Psi_0 = \Psi_0' + \sqrt{4(1-\pi^2/l^2)/3} \sin \pi x$  in Eq. (3). For Neumann boundary conditions,  $\Psi_0'(0) = \Psi_0'(1) = 0$ , the vacuum state can also be approximately obtained. The

result is

$$\Psi_0 = \begin{cases}
0, & \text{for } l \leq \pi \\
\sqrt{4(1-\pi^2/l^2)/3}\cos\pi x, & \text{for } \pi < l \leq 2\pi \\
\sqrt{4(1-\pi^2/l^2)/5 - 3/5} \pm \sqrt{8/5 - 4(1-\pi^2/l^2)/5}\cos\pi x. & \text{for } l > 2\pi
\end{cases}$$
(7)

The two solutions for  $l > 2\pi$  can be connected through  $x \leftrightarrow 1 - x$ .

Then one can consider mixed boundary conditions  $\Psi_0(0) = 0, \Psi'_0(1) = 0$ . The first order approximation of the solution for vacuum state is

$$\Psi_0(x) = \sqrt{\frac{4}{3} \left(1 - \frac{\pi^2}{4l^2}\right)} \sin\frac{\pi x}{2} \ . \tag{8}$$

As a final example, we give the vacuum state for periodic boundary condition  $\Psi_0(x) = \Psi_0(1+x)$ . The approximate vacuum state is

$$\Psi_0(x) = \begin{cases} 0, & \text{for } l \le 2\pi \\ \sqrt{4(1 - 4\pi^2/l^2)/5}(\cos 2\pi x \pm \sin 2\pi x), & \text{for } 4\sqrt{6\pi/3} \ge l > 2\pi \\ \sqrt{3(1 - 32\pi^2/3l^2)/11} \pm \sqrt{4(1 + 4\pi^2/l^2)/11}(\cos 2\pi x \pm \sin 2\pi x). & \text{for } l > 4\sqrt{6\pi/3} \end{cases}$$
(9)

It should be pointed out that  $-\Psi_0$  is also a vacuum state of the system. Then the fluctuations of the system can be around either  $\Psi_0$  or  $-\Psi_0$ . This is the copy for finite systems of spontaneous symmetry breaking in  $\phi^4$  model. With the vacuum state  $\Psi_0$ , one can shift the order parameter  $\Psi = \Psi' + \Psi_0$ , then the Hamiltonian H turns out to be

$$H = H[\Psi_0] + \frac{L^3 \phi_0^2}{\xi^2} \int d^3 x \frac{1}{2} \left[ \frac{1}{l^2} (\nabla \Psi')^2 - {\Psi'}^2 + 3\Psi_0^2 {\Psi'}^2 + 2\Psi_0 {\Psi'}^3 + \frac{1}{2} {\Psi'}^4 \right] . \tag{10}$$

In this expression,  $H[\Psi_0]$  has the same form as H in Eq. (2) with  $\Psi_0$  in place of  $\Psi$ . Now the quadratic part of fluctuation  $\Psi$  is positive definite for l larger than characteristic length, or for temperature enough below the critical point. Then one sees that the new Hamiltonian can be safely used to calculate perturbatively fluctuations at low temperature region for finite systems. For the sake of easier perturbative calculation, one can use  $\langle \Psi_0^2 \rangle$  in place of  $\Psi_0^2$ , and treat all other terms,  $H_I = \frac{L^3\phi^2}{\xi^2} \int d^3x \left[ \frac{3}{2} (\Psi_0^2 - \langle \Psi_0^2 \rangle) \Psi'^2 + \Psi_0 \Psi'^3 + \frac{1}{4} \Psi'^4 \right]$ , as small perturbations. In the lowest order, ignoring contributions from  $H_I$ , one can get one-point and two-point and other correlation functions in terms of  $\Psi_0$  and Green's function G(x,y), the inverse of operator  $-\nabla^2/l^2-1+3\langle\Psi_0^2\rangle$ . For example,

$$\langle \phi(x) \rangle = L^3 \phi_0 \Psi_0(x) \langle \phi(x) \phi(y) \rangle = L^6 \phi_0^2 (\Psi_0(x) \Psi_0(y) + \frac{\xi^2}{L^3 \phi_0^2} G(x, y))$$

$$(11)$$

For system with Dirichlet boundary conditions and under the condition that l is a little larger than  $\pi$ , the Green's function G(x,y) is

$$G(x;y) = \int \frac{d^2p}{(2\pi)^2} \sum_{i=1}^{\infty} \frac{\sin i\pi x_1 \sin i\pi y_1 e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}}{2(1-\pi^2/l^2) - (1-i^2\pi^2/l^2 - \mathbf{p}^2/l^2)}$$
(12)

Here,  $x_1, y_1$  are components of coordinates in finite size direction of two points x, y,  $\mathbf{r}$  and  $\mathbf{r}'$  are vectors in other directions,  $\mathbf{p}$  is the corresponding momentum. An important feature of the Green's function is that the translational invariance in the direction with finite length is violated. This result is natural for finite system. In this time the Green's function cannot be written as function of the difference of the coordinates of two points. The physical reason is simple. The Green's function is the response at x' of the system to a source at x. When both x and x' are translated in the same way, the influence of the boundary response changes. Thus, the net response to the source also changes. So translational invariance is surely violated. From Eq. (10) one can easily get the vertices needed. Then a perturbative calculation can be done readily, which is beyond the scope of this Letter.

In summary, we showed the importance of local spontaneous symmetry breaking for finite system in the calculation of fluctuations in phase transition in low temperature region for such system. The vacuum states are approximately given for various boundary conditions for film system within scalar  $\phi^4$  model for phase transition. With the vacuum state, perturbative calculations can be done safely.

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## Figure Caption

Fig. 1 Comparison between exact solutions and approximate ones for Eq. (3) under Dirichlet boundary conditions for  $l/\pi=1.05$ , 1.10, 1.15, and 1.20. The solid curves correspond to exact solutions, dotted curves are drawn according to Eq. (6).

